

Ethylbenzene
100-41-4 | DTXSID3020596

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 45.6

Global applicability domain: Inside

Local applicability domain index: 6.27e-01

Confidence level: 8.36e-01

Nearest Neighbors from the Training Set

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5-Ethylidene-2-norbornene

Measured: 110

Predicted: 134

Image not found

4-Vinylcyclohexene

Measured: 166

Predicted: 158

Image not found

1,2-Dibromoethane

Measured: 15.1

Predicted: 13.4

Image not found

Bromobenzene

Measured: 22.9

Predicted: 11.7

Image not found

Thiophene, 3-methyl-

Measured: 5.25

Predicted: 7.49